SOFT MATTER

A SELF-CONSISTENT MICROSCOPIC MODEL OF THE ENERGY SPECTRUM OF SUPERFLUID ⁴He WITH THE HERMITIAN FORM OF THE BOGOLYUBOV–ZUBAREV HAMILTONIAN

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Based on the representation of collective variables with the Hermitian form of the Bogolyubov-Zubarev Hamiltonian, a self-consistent oscillator model of the ground state and excited states of a Bose liquid has been proposed. A new method of calculation of anharmonic terms in this Hamiltonian and its interpretation have been presented. The dispersion equation for a collective excitation in superfluid ${}^{4}\mathrm{He}$ has been obtained in a self-consistent way, where the real and virtual processes of decay of a collective excitation are considered. The end point, which is determined by the threshold of collective excitation's decay into two rotons, of the dispersion curve has been obtained, and it is shown that the dispersion curve strongly depends on the property of its stability. An approach with a structure factor has been realized without use of any fitting parameters. Based on the oscillator model, a new method of selfconsistent calculation of the ground-state energy and the density of a Bose condensate has been proposed. The model of suppression of a Bose condensate has been presented.

1. Introduction

Up to the present time, many various models have been proposed for the microscopic description of superfluid helium. Most of the models are based on two approaches. The first one is the field-theoretic formalism. Its characteristic feature is the explicit application of a Bosecondensate (BC) and the introduction of the higher BC in some models [1–4]. The second one is the quantummechanical approach, where the Schrödinger equation is solved for the ground state and for the lowest excited states of N interacting particles. This approach originates from the papers of Feynman and Cohen [5], where the connection between the structure factor and the dispersion curve of collective excitations (CE) was obtained. However, this connection is correct at small values of a wave vector only $(k \rightarrow 0)$. The quantum-mechanical approach does not use BC explicitly unlike the field-theoretic approach, but it calculates BC knowing the ground-state wave function.

The quantum-mechanical approach has been developed essentially due to the use of the Bogolyubov-Zubarev formalism [6]. In this representation, the Hamiltonian of a system of bosons is written in the terms of $\rho_{\mathbf{k}}$ and $\partial/\partial \rho_{\mathbf{k}}$, where $\rho_{\mathbf{k}}$ is a Fourier transform of the density fluctuation. As it has been shown in papers [7, 8], the normal motion and the superfluid motion can be separated in the N-particle Schrödinger equation. The oscillations of a Bose liquid are obtained in the harmonic approximation. Zero-point oscillations correspond to the ground state of the liquid, and excited states – to any collective excitations: phonons, rotons, maxons, and so on. However, the non-harmonic terms of the Hamiltonian play an essential role. The first correction to the harmonic approximation has been calculated in the above-mentioned papers, and the second correction has been calculated in paper [9]. Unfortunately, no small parameters are in this expansion and the calculation of each new correction is accompanied by large mathematical difficulties. The contribution of anharmonic terms to the energy of a liquid has been evaluated by the Brillouin-Wigner perturbation procedure in papers [10, 11]. We mention also the application of the method of Green function [12] and the "shadow wave function" approach [13].

The dispersion curve of CE obtained by some authors [5, 9–11] coincides satisfactorily with the experimental spectrum, if the value of wave vector is $k < 2.5 \text{ Å}^{-1}$. In the region k > 3 Å⁻¹, the experimental spectrum reaches the "shelf," i.e., a hybridization of CE with the two-roton level is observed [14]. The region $k > 3 \text{ Å}^{-1}$ has been investigated by the field-theoretic method in [15], where it was shown that the "shelf" on the dispersion curve is caused by the decay of CE into two rotons and by the end of the spectrum. The calculation of next corrections to the spectrum of CE doesn't give the end point of a dispersion curve. We have to note that the potential of interaction between atoms is known badly on small distances r < 2.5 Å. The ground-state energy is very sensitive to the interaction at small distances just. The situation is complicated by the facts that He II is a liquid, and no complete theory of liquid was developed till now. That's why the authors proceed from the gas representation or the models of quantum crystal [16-18].

The Bogolyubov-Zubarev Hamiltonian is non-Hermitian because the transition from Cartesian coordinates to the collective coordinates is non-unitary. This Hamiltonian has been used in the many aforesaid papers [6-9, 12, 19-22]. But the non-Hermiticity must lead to the violation of some theorems of quantum mechanics. However, the operator of speed $g_{\mathbf{k}}$ canonically conjugated with $\rho_{\mathbf{k}}$ has been introduced in paper [10], and the Hamiltonian represented by these terms is Hermitian. The Hermitian form of the Bogolyubov-Zubarev Hamiltonian and the Jacobian of the transition to collective coordinates have been obtained in book [23]. However, the anharmonic terms of this Hamiltonian have not been calculated.

In Section 2, the superfluid motion and the normal motion are separated in the Schrödinger equation with the Hermitian form of the Bogolyubov-Zubarev Hamiltonian. In Section 3, the oscillator model of Bose liquid has been formulated in the Random Phase Approximation (RPA). In Section 4, the contribution of anharmonic terms of the Hamiltonian to the spectrum of CE has been calculated. It has been shown that this correction describes the decay of CE, and the dispersion curve has the end point $k_{\rm C}$. In Section 5, the ground-state energy E_0 has been calculated with regard for anharmonic terms in the Hamiltonian with the help of the oscillator model. The mechanism of suppression of BC has been described, and the density of BC at zero temperature has been calculated.

2. The Equation of Motion and the Space of Collective Variables

Let us consider N interacting Bose particles of mass m confined in a macroscopic volume V. The Hamiltonian of the system has the form

$$\hat{H} = \sum_{1 \le j \le N} \frac{\hat{p}^2}{2m} + \sum_{1 \le i < j \le N} \Phi(|\mathbf{r}_i - \mathbf{r}_j|), \tag{1}$$

where \hat{p} is the operator of momentum of a particle, and the operator $\Phi(|\mathbf{r}_i - \mathbf{r}_j|)$ is the energy of interaction of two particles, and describes oscillations of a Bose liquid. The waves functions must be symmetric for any rearrangements of coordinates of any pairs from N particles. The space of the collective variables is the suitable multitude of variables describing the collective motion of a system [24, 25]. Collective variables are the Fourier transform of fluctuations of the density $\Delta n(\mathbf{r}) = \sum_{j=1}^{N} \delta(\mathbf{r} - \mathbf{r}_j) - N/V$:

$$\rho_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} \exp(-i\mathbf{k}\mathbf{r}) = \rho_{\mathbf{k}}^{c} - i\rho_{\mathbf{k}}^{s}, \qquad (2)$$

where

$$\rho_{\mathbf{k}}^{c} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} \cos(\mathbf{k}\mathbf{r}), \qquad \rho_{\mathbf{k}}^{s} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} \sin(\mathbf{k}\mathbf{r}).$$
(3)

What's more, the correlations have a place:

$$\rho_{\mathbf{k}}^* = \rho_{-\mathbf{k}} \qquad \Rightarrow \qquad \rho_{\mathbf{k}}^c = \rho_{-\mathbf{k}}^c, \qquad \rho_{\mathbf{k}}^s = -\rho_{-\mathbf{k}}^s. \tag{4}$$

This means that it is necessary to consider the values $\rho_{\mathbf{k}}$ with indices \mathbf{k} from the half-space of their possible values only.

The transition from the Cartesian coordinates $(\mathbf{r}_1, ..., \mathbf{r}_N)$ to the variables $\rho_{\mathbf{k}}$ is nonunitary, because the number of the Cartesian coordinates is 3N, but the number of $\rho_{\mathbf{k}}$ -variables is infinity. Hence, superfluous variables exist among collective variables. The transition to the $\rho_{\mathbf{k}}$ -representation must be done with the Jacobian which equalizes the volume of the configuration space $\int d\mathbf{r}_1 \dots \int d\mathbf{r}_N = V^N$ to the volume of the $\rho_{\mathbf{k}}$ -space:

$$V^{N} = \prod_{\mathbf{k}\neq 0}^{\prime} \int_{-\sqrt{N}}^{\sqrt{N}} d\rho_{\mathbf{k}}^{c} \int_{-\sqrt{N}}^{\sqrt{N}} d\rho_{\mathbf{k}}^{s} J,$$
(5)

where the prime at the symbol of multiplication means that the variables \mathbf{k} are taken from the half-space only.

ISSN 2071-0194. Ukr. J. Phys. 2011. Vol. 56, No. 11

In the representation of new variables (2), Hamiltonian (1) has the form

$$\hat{H}_{\rm BZ} = \sum_{\mathbf{k}_1 \neq 0} \varepsilon(k_1) \left(\rho_{\mathbf{k}_1} \frac{\partial}{\partial \rho_{\mathbf{k}_1}} - \frac{\partial^2}{\partial \rho_{\mathbf{k}_1} \partial \rho_{-\mathbf{k}_1}} \right) + \\ + \sum_{\mathbf{k}_1 \neq 0} \sum_{\mathbf{k}_2 \neq 0}^{\mathbf{k}_1 + \mathbf{k}_2 \neq 0} \frac{\varepsilon(\mathbf{k}_1, \mathbf{k}_2)}{\sqrt{N}} \rho_{\mathbf{k}_1 + \mathbf{k}_2} \frac{\partial^2}{\partial \rho_{\mathbf{k}_1} \partial \rho_{\mathbf{k}_2}} + \\ + \frac{N^2}{2V} \nu(0) + \frac{N}{2V} \sum_{\mathbf{k}_1 \neq 0} \nu(k_1) \left(\rho_{\mathbf{k}_1} \rho_{-\mathbf{k}_1} - 1 \right), \tag{6}$$

and is called the Bogolyubov–Zubarev Hamiltonian. However, this operator is non-Hermitian – the first term in the first brackets: $\rho_{\mathbf{k}_1} \frac{\partial}{\partial \rho_{\mathbf{k}_1}}$. This property of \hat{H}_{BZ} is caused by the nonunitary transition from Cartesian variables to collective ones $\rho_{\mathbf{k}}$.

The Hermitian form of Hamiltonian (6) has been obtained in paper [23]. Let the system be described by the wave function ψ , which is normalized in the $\rho_{\mathbf{k}}$ representation:

$$\prod_{\mathbf{k}\neq 0}^{\prime} \int_{-\sqrt{N}}^{\sqrt{N}} d\rho_{\mathbf{k}}^{c} \int_{-\sqrt{N}}^{\sqrt{N}} d\rho_{\mathbf{k}}^{s} J |\psi|^{2} = 1.$$
(7)

We now introduce the wave functions normalized without the Jacobian J:

$$\bar{\psi} = \psi \sqrt{J}.\tag{8}$$

Then the Schrödinger equation can be written as follows:

$$\hat{H}\bar{\psi} = E\bar{\psi}, \qquad \hat{H} = J^{1/2}\hat{H}_{\rm BZ}J^{-1/2},$$
(9)

where the new Hamiltonian \hat{H} must be Hermitian. Proceeding from this condition, we can find the Jacobian J. Then we have

$$\begin{split} \hat{H} &= \sum_{\mathbf{k}_1 \neq 0} \varepsilon(k_1) \left(-\frac{\partial^2}{\partial \rho_{\mathbf{k}_1} \partial \rho_{-\mathbf{k}_1}} - \frac{1}{4} \rho_{\mathbf{k}_1} \frac{\partial \ln J}{\partial \rho_{\mathbf{k}_1}} - \frac{1}{2} \right) + \\ &+ \sum_{\mathbf{k}_1 \neq 0} \sum_{\mathbf{k}_2 \neq 0}^{\mathbf{k}_1 + \mathbf{k}_2 \neq 0} \frac{\varepsilon(\mathbf{k}_1, \mathbf{k}_2)}{\sqrt{N}} \rho_{\mathbf{k}_1 + \mathbf{k}_2} \frac{\partial^2}{\partial \rho_{\mathbf{k}_1} \partial \rho_{\mathbf{k}_2}} + \end{split}$$

$$+\frac{N^2}{2V}\nu(0) + \frac{N}{2V}\sum_{\mathbf{k}_1\neq 0}\nu(k_1)\left(\rho_{\mathbf{k}_1}\rho_{-\mathbf{k}_1} - 1\right),\tag{10}$$

where the Jacobian must be found from the equation:

$$\rho_{\mathbf{k}_1} + \frac{\partial \ln J}{\partial \rho_{-\mathbf{k}_1}} - \frac{1}{\sqrt{N}} \sum_{\mathbf{k}_1 \neq 0}^{\mathbf{k}_1 + \mathbf{k}_2 \neq 0} \frac{\mathbf{k}_1 \mathbf{k}_2}{k_1^2} \rho_{\mathbf{k}_1 + \mathbf{k}_2} \frac{\partial \ln J}{\partial \rho_{\mathbf{k}_2}} = 0.$$
(11)

The solution of this equation reads

$$\ln J = \ln C + \sum_{n \ge 2} \frac{(-1)^{n-1}}{n(n-1)(\sqrt{N})^{n-2}} \sum_{\mathbf{q}_1 \ne 0} \dots \sum_{\mathbf{q}_n \ne 0} \rho_{\mathbf{q}_1} \dots \rho_{\mathbf{q}_n}.$$
(12)

The constant C can be found from condition (5). In our comprehension, Eq. (9) with Hamiltonian (10) is the *motion equation* in the $\rho_{\mathbf{k}}$ -space. Equation (11) is the *constraint equation* in this space. In Cartesian coordinates, we have a discrete system of N particles. But, in collective coordinates, the system is regarded as a continuum. The constraint equation removes the superfluous degrees of freedom.

The normal motion and the superfluid motion can be separated in the Schrödinger equation [7]. The wave function of the ground state describes zero-point oscillations of the Bose liquid and has an exponential form e^{U} . The whole wave function (with excited states) has the form

$$\bar{\psi} = e^U \varphi. \tag{13}$$

Then we rewrite the energy of the fluid as

$$E = E_0 + E - E_0 \equiv E_0 + E_{\text{ext}},$$
 (14)

where E_0 is the ground-state energy (energy of superfluid motion with the wave function e^U), E_{ext} is the energy of excitation (energy of normal motion with the wave function φ). Then Eq. (9) is divided into the set of equations describing the superfluid motion

$$-\sum_{\mathbf{k}_{1}\neq0}\varepsilon(k_{1})\left[\frac{\partial^{2}U}{\partial\rho_{\mathbf{k}_{1}}\partial\rho_{-\mathbf{k}_{1}}}+\frac{\partial U}{\partial\rho_{\mathbf{k}_{1}}}\frac{\partial U}{\partial\rho_{-\mathbf{k}_{1}}}\right]+$$

$$+\sum_{\mathbf{k}_{1}\neq0}\sum_{\mathbf{k}_{2}\neq0}\frac{\varepsilon(\mathbf{k}_{1},\mathbf{k}_{2})}{\sqrt{N}}\rho_{\mathbf{k}_{1}+\mathbf{k}_{2}}\left[\frac{\partial U}{\partial\rho_{\mathbf{k}_{1}}\partial\rho_{\mathbf{k}_{2}}}+\frac{\partial U}{\partial\rho_{\mathbf{k}_{1}}}\frac{\partial U}{\partial\rho_{\mathbf{k}_{2}}}\right]+$$

$$+\sum_{\mathbf{k}_{1}\neq0}\left[\frac{N}{2V}\nu(k_{1})\rho_{\mathbf{k}_{1}}\rho_{-\mathbf{k}_{1}}-\frac{1}{4}\rho_{\mathbf{k}_{1}}\frac{\partial\ln J}{\partial\rho_{\mathbf{k}_{1}}}\varepsilon(k_{1})\right]=$$

$$=E_{0}+\sum_{\mathbf{k}\neq0}\left[\frac{1}{2}\varepsilon(k)+\frac{N}{2V}\nu(k)\right]-\frac{N^{2}}{2V}\nu(0)$$
(15)

ISSN 2071-0194. Ukr. J. Phys. 2011. Vol. 56, No. 11

and the normal motion

$$-\sum_{\mathbf{k}_{1}\neq0}\varepsilon(k_{1})\left[\frac{\partial^{2}\varphi}{\partial\rho_{\mathbf{k}_{1}}\partial\rho_{-\mathbf{k}_{1}}}+2\frac{\partial U}{\partial\rho_{\mathbf{k}_{1}}}\frac{\partial\varphi}{\partial\rho_{-\mathbf{k}_{1}}}\right]+$$
$$+\sum_{\mathbf{k}_{1}\neq0}\sum_{\mathbf{k}_{2}\neq0}\frac{\varepsilon(\mathbf{k}_{1},\mathbf{k}_{2})}{\sqrt{N}}\rho_{\mathbf{k}_{1}+\mathbf{k}_{2}}\left[\frac{\partial\varphi}{\partial\rho_{\mathbf{k}_{1}}}\partial\rho_{\mathbf{k}_{2}}}+2\frac{\partial U}{\partial\rho_{\mathbf{k}_{1}}}\frac{\partial\varphi}{\partial\rho_{\mathbf{k}_{2}}}\right]=$$
$$=E_{\mathrm{ext}}(k)\varphi.$$
(16)

The wave function ψ must be an eigenfunction of the momentum operator [7,8]:

$$\hat{\mathbf{P}} = -\sum_{\mathbf{k}_1 \neq 0} \hbar \mathbf{k}_1 \rho_{\mathbf{k}_1} \frac{\partial}{\partial \rho_{\mathbf{k}_1}}, \qquad \hat{\mathbf{P}} \psi = \mathbf{P} \psi.$$
(17)

The wave function $\bar{\psi}$ is an eigenfunction of the momentum operator as well:

$$J^{1/2}\hat{\mathbf{P}}J^{-1/2}\bar{\psi} = \mathbf{P}\bar{\psi} \Longrightarrow \hat{\mathbf{P}}\bar{\psi} = \mathbf{P}\bar{\psi}.$$
 (18)

The proof of this fact is in Appendix 6. Then the solution of Eqs. (15) and (16) must obey the condition

$$\hat{\mathbf{P}}e^U = 0 \cdot e^U, \qquad \hat{\mathbf{P}}\varphi = \hbar(\mathbf{k}_1 + \ldots + \mathbf{k}_n)\varphi.$$
 (19)

This means that the center of masses of the system rests, and the function φ describes excited states of a system, which are characterized by the conserved energy $E_{\text{ext}}(k)$ and the conserved momentum $\hbar(\mathbf{k}_1 + \ldots + \mathbf{k}_n)$. Thus, the function φ describes the state with *n* collective excitations. If the interaction of particles is absent, $\nu(k) = 0$, then the wave function ψ is a wave function of free bosons $\psi_{\nu=0} = 1/\sqrt{V^N}$. A proof of this statement is in Appendix 6.

In the general case, a solution of Eq. (15) has the form of a correlation series expansion [7, 8]:

$$U = \sum_{\mathbf{k}\neq 0} f(k)\rho_{\mathbf{k}}\rho_{-\mathbf{k}} + \sum_{\mathbf{k}\neq 0} \sum_{\mathbf{q}\neq 0}^{\mathbf{k}+\mathbf{q}\neq 0} \frac{g(\mathbf{k},\mathbf{q})}{\sqrt{N}}\rho_{\mathbf{q}-\mathbf{k}}\rho_{\mathbf{k}}\rho_{-\mathbf{q}} + \dots$$
(20)

An analogous expansion for the function φ of the state with one CE (as $\hat{\mathbf{P}}\varphi = \hbar \mathbf{k}\varphi$) has the form

$$\varphi = \rho_{-\mathbf{k}} + \sum_{\mathbf{q}\neq 0}^{\mathbf{k}+\mathbf{q}\neq 0} \frac{L(\mathbf{k},\mathbf{q})}{\sqrt{N}} \rho_{\mathbf{q}-\mathbf{k}}\rho_{-\mathbf{q}} + \dots$$
(21)

Unfortunately, no small parameter exists in these expansions. What's more, the calculation of higher terms

ISSN 2071-0194. Ukr. J. Phys. 2011. Vol. 56, No. 11

of the expansions is very difficult mathematically. In order to solve this problem, we have to use some model considerations and approximations.

We have to make a little remark here. Under *collective excitations*, we understand the quanta of collective motions of a macroscopic group of particles, i.e., the motion of system as a whole. For example: phonon, plasmon, magnon. Under a *quasiparticle*, we understand a particle interacting with its environment or an external field ("dressed" particle). The quasiparticles are characterized by the effective mass, and they interact with effective (screened) potential. The examples of quasiparticles are conduction electrons, polarons, Cooper pairs.

3. Random Phase Approximation

3.1. The random phases as zeroth approximation

In this section, we will shortly formulate the zeroth approximation to our problem – RPA or harmonic approximation. We write the Jacobian and the ground-state wave function in the Gauss form:

$$\ln J = \ln C - \frac{1}{2} \sum_{\mathbf{k} \neq 0} \rho_{\mathbf{k}} \rho_{-\mathbf{k}}.$$
(22)

$$U = \sum_{\mathbf{k}\neq 0} f(k)\rho_{\mathbf{k}}\rho_{-\mathbf{k}}.$$
(23)

Substituting these expressions in Eq. (15) and neglecting the powers of $\rho_{\mathbf{k}}$ higher than the second one, we have

$$\sum_{\mathbf{k}\neq 0} \left[-4\varepsilon(k)f^2(k) + \frac{1}{4}\varepsilon(k) + \frac{N}{2V}\nu(k) \right] \rho_{\mathbf{k}}\rho_{-\mathbf{k}} = E_0 - \frac{1}{2V}\rho_{\mathbf{k}}\rho_{-\mathbf{k}} = E_0 - \frac{1}{2V}\rho_{\mathbf{k}}\rho_{-\mathbf{k}}$$

$$-\frac{N^2}{2V}\nu(0) + \sum_{\mathbf{k}\neq 0} \left[2\varepsilon(k)f(k) + \frac{1}{2}\varepsilon(k) + \frac{N}{2V}\nu(k) \right].$$
(24)

From this equation, we can obtain the unknown function f,

$$f(k) = -\frac{1}{4}\sqrt{1 + \frac{2N}{V}\frac{\nu(k)}{\varepsilon(k)}},\tag{25}$$

and the corresponding energy

$$E_0 = \sum_{\mathbf{k} \neq 0} \frac{1}{2} \sqrt{\varepsilon(k)^2 + \frac{2N}{V} \nu(k)\varepsilon(k)} -$$

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$$-\sum_{\mathbf{k}\neq 0} \left[\frac{1}{2} \varepsilon(k) + \frac{N}{2V} \nu(k) \right] + \frac{N^2}{2V} \nu(0).$$
(26)

We note that solutions (25 and 26) correspond to the truncated Hamiltonian

$$\hat{H}_{\text{RPA}} = \sum_{\mathbf{k}_1 \neq 0} \varepsilon(k_1) \left(-\frac{\partial^2}{\partial \rho_{\mathbf{k}_1} \partial \rho_{-\mathbf{k}_1}} + \frac{1}{4} \rho_{\mathbf{k}_1} \rho_{-\mathbf{k}_1} - \frac{1}{2} \right) +$$

$$+\frac{N^2}{2V}\nu(0) + \frac{N}{2V}\sum_{\mathbf{k}_1\neq 0}\nu(k_1)\left(\rho_{\mathbf{k}_1}\rho_{-\mathbf{k}_1} - 1\right),$$
(27)

where, unlike the complete Hamiltonian (10), the harmonic terms are kept only.

A structure factor is the most important characteristic of liquids [24]:

$$S(k) = \langle \rho_{\mathbf{k}} \rho_{-\mathbf{k}} \rangle. \tag{28}$$

Here, the mean value $\langle \rangle$ is calculated with the ground state. This function can be obtained by using the virial theorem:

$$\frac{\delta E}{\delta \nu(k)} = \left\langle \frac{\delta \hat{H}}{\delta \nu(k)} \right\rangle \Rightarrow S(k) = -\frac{1}{4f(k)}.$$
(29)

For atoms of helium, the potential of interaction is very like to the Lennard-Jones potential in the region r > 2.5 Å. In the remaining region, the interaction is known badly, and various adaption functions have be used here. In order to get over this difficulty, the approach with a structure factor has been developed in some papers, where the potential of interaction is the unknown function, and the structure factor is taken from experimental data. This means that the perturbation theory must be constructed, so we must obtain the same structure factor in each approximation. On the present step of calculations, the potential of interaction is obtained from (29) in the form

$$\nu(k) = \frac{V}{2N}\varepsilon(k) \left[\frac{1}{S^2(k)} - 1\right].$$
(30)

In order to obtain the dispersion curve of a CE, we assume that $\varphi = \rho_{-\mathbf{k}}$. Substituting it and function (23) in Eq. (16), we have

$$E_{\text{ext}}^{\text{RPA}} = \frac{\varepsilon(k)}{S(k)} = \sqrt{\varepsilon(k)^2 + \frac{2N}{V}\nu(k)\varepsilon(k)}.$$
(31)

This expression is known as the Feynman formula or the Bogolyubov spectrum. Formula (31) is a starting-point in order to obtain the dispersion curve of a CE which is consistent with the experimental spectrum.

3.2. Formulation of the oscillator model

Hamiltonian (27) is a sum of separate terms, where each of them is characterized by the own wave vector **k**. This fact means that the infinite number of independent motions can be in the system, and every of them is characterized by a wave vector **k** and some energy $\xi(k)$. For each independent motion, the Schrödinger equation is written as follows:

$$-\frac{\hbar^2}{2(m/k^2)}\frac{\partial^2\bar{\psi}}{\partial\rho_{\mathbf{k}}\partial\rho_{-\mathbf{k}}} + \left[\frac{1}{4}\varepsilon(k) + \frac{N}{2V}\nu(k)\right]\rho_{\mathbf{k}}\rho_{-\mathbf{k}}\bar{\psi} =$$
$$= \xi(k)\bar{\psi}.$$
(32)

This equation is similar to the equation of a harmonic oscillator, where

$$M \equiv \frac{m}{k^2}, \qquad \frac{1}{4}\varepsilon(k) + \frac{N}{2V}\nu(k) \equiv \frac{1}{2}M\omega^2.$$
(33)

The energy of an oscillator with the wave vector ${\bf k}$ is

$$\xi(k) = \hbar\omega(k)\left(\frac{1}{2} + n\right) = \frac{\varepsilon(k)}{S(k)}\left(\frac{1}{2} + n\right),\tag{34}$$

and the ground-state energy of the system is

$$E_{0} = \sum_{\mathbf{k}\neq 0} \frac{1}{2} \hbar \omega(k) - \sum_{\mathbf{k}\neq 0} \left[\frac{1}{2} \varepsilon(k) + \frac{N}{2V} \nu(k) \right] + \frac{N^{2}}{2V} \nu(0).$$
(35)

The wave function of the ground state has the form

$$\bar{\psi} \sim \exp\left(-\frac{\rho_{\mathbf{k}}\rho_{-\mathbf{k}}}{2l^2}\right) = e^{f(k)\rho_{\mathbf{k}}\rho_{-\mathbf{k}}}, \qquad l^2 = \frac{\hbar}{M\omega}$$
(36)

where l is a oscillator length. The structure factor can be found from the virial theorem for an oscillator:

$$\frac{M\omega^2}{2}\langle \rho_{\mathbf{k}}\rho_{-\mathbf{k}}\rangle = \frac{\xi(k)}{2} \Rightarrow S = \frac{\varepsilon(k)}{\hbar\omega(k)}[1+2\langle n\rangle], \qquad (37)$$

and the state n = 0 corresponds to the ground state. The structure factor S(k) is the dispersion of a oscillator with a wave vector **k**.

Based on the aforesaid assumptions, we can formulate the oscillator model of a Bose liquid. The quantum liquid represents a totality of harmonic oscillators. Each oscillator is a vibration mode of the liquid density. The ground-state energy of the system is a sum of the energies of ground states of these oscillators. The presence

ISSN 2071-0194. Ukr. J. Phys. 2011. Vol. 56, No. 11

of n collective excitations in a system corresponds to a state with n excited oscillators. The oscillator model is a model of continuum medium, and it is incorrect at distances between neighboring atoms. The calculation of short-range correlations is very difficult, because all anharmonic terms in Hamiltonian (10) and in Jacobian (12) must be calculated. Moreover, if we try to calculate them with the help of ordinary perturbation theory, then we have divergent integrals. This difficulty appears due to the contribution of the above-mentioned superfluous degrees of freedom. In the next sections, we formulate the method of calculation of the anharmonic terms, by remaining in the limits of the oscillator model.

4. The Spectrum of Collective Excitations

4.1. Decay of collective excitations

The wave function of an excited state $\varphi = \rho_{-\mathbf{k}}$ leads to the well-known Feynman formula (31). In Fig.1, we can see that the dispersion curve in RPA coincides with the experimental dispersion curve in the limit $k \to 0$ only. Its basic contrast to the real spectrum is that the Feynman formula doesn't involve the decay of a CE and the end of a dispersion curve.

Let's consider the wave function of a CE (21) with momentum $\hbar \mathbf{k}$, where $L(\mathbf{k}, \mathbf{q})$ is the unknown function. In our interpretation, the second term in (21) describes the process of decay of a CE with momentum $\hbar \mathbf{k}$ and energy $E_{\text{ext}}(k)$ into two excitations with momenta $\hbar(\mathbf{k} - \mathbf{q})$ and $\hbar \mathbf{q}$ and with energies $E_{\text{ext}}(|\mathbf{k} - \mathbf{q}|)$ and $E_{\text{ext}}(q)$, respectively. Decay of CE can occur if energy is conserved:

$$E_{\text{ext}}(k) = E_{\text{ext}}(|\mathbf{k} - \mathbf{q}|) + E_{\text{ext}}(q).$$
(38)

Such a situation corresponds to case (A) in Fig. 2. This process causes the damping of a CE and the end of the dispersion curve [26]. In those parts of the energy spectrum where equality (38) isn't true, CE is stable. In this case, the term in (21) with the multiplier $\rho_{\mathbf{q}-\mathbf{k}}\rho_{-\mathbf{q}}$ describes the processes of virtual decay and creation of CE. This causes the trivial renormalization of the energy spectrum of CE. This situation corresponds to case (B) in Fig. 2. Higher approximations in (21) describe decays of CE into three and more excitations. We suppose that such processes are improbable, and we will not consider them in this paper.

Substituting the wave function (21) in Eq. (16), we obtain the function

$$L(\mathbf{k}, \mathbf{q}) = \frac{\varepsilon(\mathbf{k}, \mathbf{q})S^{-1}(q)}{E_{\text{ext}}(k) - E_{\text{ext}}^{\text{RPA}}(|\mathbf{k} - \mathbf{q}|) - E_{\text{ext}}^{\text{RPA}}(q)}, \qquad (39)$$

ISSN 2071-0194. Ukr. J. Phys. 2011. Vol. 56, No. 11

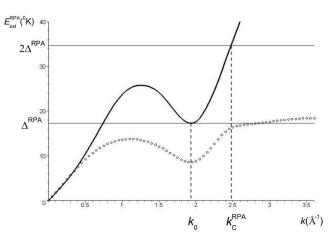


Fig. 1. Spectrum of CE calculated with the Feynman formula (solid line) and measured in experiment (dotted line). Decay of a excitation into two rotons is possible in the region $k > k_{\rm C}^{\rm RPA}$, where $E_{\rm ext}^{\rm RPA}(k) > 2\Delta^{\rm RPA}$. The experimental curve has a "shelf" at k > 2.5 Å⁻¹, where the decay of CE into two rotons is observed

where $E_{\text{ext}}^{\text{RPA}}(q)$ is the spectrum of CE in RPA – formula (31). In addition, we obtain the dispersion law of CE in the form

$$E_{\text{ext}}(k) = E_{\text{ext}}^{\text{RPA}}(k) + \frac{2}{N} \sum_{\mathbf{q} \neq 0} L\varepsilon(\mathbf{k} - \mathbf{q}, \mathbf{q}) = E_{\text{ext}}^{\text{RPA}}(k) -$$

$$-\frac{2}{N}\sum_{\mathbf{q}\neq 0}\frac{\varepsilon(\mathbf{k},\mathbf{q})\varepsilon(\mathbf{k}-\mathbf{q},\mathbf{q})S^{-1}(q)}{E_{\mathrm{ext}}^{\mathrm{RPA}}(|\mathbf{k}-\mathbf{q}|) + E_{\mathrm{ext}}^{\mathrm{RPA}}(q) - E_{\mathrm{ext}}(k)}.$$
(40)

This equation is an integral equation for the unknown function $E_{\text{ext}}(k)$. The first term corresponds to the term $\rho_{-\mathbf{k}}$ in the wave function (21), and it is the Bogolyubov–Feynman spectrum. The second term has a singularity in those points q, where the equality

$$E_{\text{ext}}(k) = E_{\text{ext}}^{\text{RPA}}(|\mathbf{k} - \mathbf{q}|) + E_{\text{ext}}^{\text{RPA}}(q)$$
(41)

holds. This relation reminds expression (38), and it is the condition for the decay of CE. The inaccuracy of this condition is in that a real CE $E_{\text{ext}}(k)$ decays into excitations with a spectrum calculated in RPA: $E_{\text{ext}}^{\text{RPA}}(q)$. However, in the region of large q, the theoretical dispersion law of CE differs from the real law $E_{\text{ext}}(q)$ essentially. We shall get over this difficulty later. For the present, we shall work with condition (41).

CE is stable at those k, where Eq. (41) has no solutions. The damping of CE appears at the decay threshold $k = k_{\rm C}$. At the point $k = k_{\rm C}$, a solution of Eq. (41) appears at first, and the right-hand sides of Eqs. (38) and (41) have extremum [26] as a function of q. We

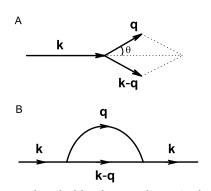


Fig. 2. Processes described by the second term in the wave function (21). Process (A) is a real decay, and process (B) is a virtual decay of CE with momentum $\hbar \mathbf{k}$ into two excitations with momenta $\hbar (\mathbf{k} - \mathbf{q})$ and $\hbar \mathbf{q}$

can see in Fig. 1 that the extremum for the function $E_{\text{ext}}^{\text{RPA}}(q)$ is the roton minimum. In its neighborhood, the spectrum of collective excitations is as follows:

$$E_{\rm ext}^{\rm RPA}(q) = \Delta^{\rm RPA} + \frac{\hbar^2}{2\mu} (q - k_0)^2, \qquad (42)$$

$$E_{\text{ext}}^{\text{RPA}}(|\mathbf{k} - \mathbf{q}|) = \Delta^{\text{RPA}} + \frac{\hbar^2}{2\mu}(|\mathbf{k} - \mathbf{q}| - k_0)^2.$$
(43)

Here, $\Delta^{\text{RPA}}=17.3$ K is the roton gap in RPA (in degrees of Kelvin), $\mu = 0.09 \ m$ is the effective mass of a roton in RPA, k_0 is momentum corresponding to the roton gap. We can suppose that $k_0 = k_0^{\text{RPA}} = 1.93 \ \text{Å}^{-1}$ in all approximations. Condition (41) is executed when $E_{\text{ext}}(k) = 2\Delta^{\text{RPA}}$. Then the integrand in spectrum (40) at $k = k_{\text{C}}$ has a singularity at the point $q = q_0$. This means the decay of CE with momentum $\hbar k_{\text{C}}$ into two rotons with momenta $\hbar k_0$ each. Hence, we have the connection $k_{\text{C}} = 2k_0 \cos \theta_c$, where $2\theta_c$ is the angle of recession of two rotons.

Let's evaluate the integral in (40) at the point $k = k_{\rm C}$. We consider the asymptotics of the integrand as $q \to \infty$, where $S(q) \to 1$. If the vector **k** is directed along the axis Oz, then $\mathbf{kq} = kq \cos \theta$. Let's use expressions (42) and (43) in the denominator of (40), as they determine the singularity at $q = k_0$, and we have $|\mathbf{k} - \mathbf{q}| \approx q$. Then the integral in (40) can be written in the form

$$\frac{2}{N} \frac{V}{(2\pi)^3} \left(\frac{\hbar^2}{2m}\right)^2 \left(\int \frac{(qk\cos\theta)^2 q^2 dq\sin\theta d\theta d\varphi}{2\Delta^{\text{RPA}} - E_{\text{ext}} + \frac{\hbar^2}{\mu} (q - k_0)^2} - \int \frac{qk\cos\theta q^2 q^2 dq\sin\theta d\theta d\varphi}{2\Delta^{\text{RPA}} - E_{\text{ext}} + \frac{\hbar^2}{\mu} (q - k_0)^2}\right) =$$
(44)

$$=\frac{4}{3N}\frac{V}{(2\pi)^2}\left(\frac{\hbar^2}{2m}\right)^2k^2\int\frac{q^4dq}{2\Delta^{\text{RPA}}-E_{\text{ext}}+\frac{\hbar^2}{\mu}(q-k_0)^2}.$$
(45)

In the second integral in (44), the integration over θ gives zero. In view of the equality $E_{\text{ext}}(k_{\text{C}}) = 2\Delta^{\text{RPA}}$, we can rewrite (45) as

$$\frac{4}{3N} \frac{V}{(2\pi)^2} \left(\frac{\hbar^2}{2m}\right)^2 k^2 \frac{\mu}{\hbar^2} \int_0^\infty \frac{q^4}{(q-k_0)^2} dq \to \infty.$$
(46)

The integrand has a pole at the point k_0 , which results in some complex addendum to the energy of CE: $E_{\text{ext}} - i/\tau$. This means the damping and the bounded lifetime $\sim \tau$ of CE. Moreover, we can see that the *ultraviolet divergence* takes place. Hence, the second term in formula (40) for the spectrum of CE tends to infinity: $E_{\text{ext}}(k) = E_{\text{ext}}^{\text{RPA}}(k) + \infty$. The nature of this divergence lies in the following.

The constraint equation (11) removes the superfluous degrees of freedom appeared at the nonunitary transition to collective coordinates. These degrees of freedom are connected with the continuum representation of a primarily discrete medium. Each superfluous degree of freedom gives contribution to the energy. The neglect of all anharmonic terms in Jacobian (12) and in Hamiltonian (10) doesn't give possibility to delete this nonphysical energy. The contribution of the superfluous degrees of freedom results in a singularity in integral (40).

The method of removal of the divergence is the cutoff of integral (40) to some unknown value of the wave vector $q = q_m$. By analogy with [15, 26], we introduce new variables q'_z II q'_ρ in accordance with the definition:

$$q_{x} = (k_{0} \sin \theta_{c} + q'_{\rho}) \cos \varphi,$$

$$q_{y} = (k_{0} \sin \theta_{c} + q'_{\rho}) \sin \varphi,$$

$$q_{z} = k_{0} \cos \theta_{c} + q'_{z},$$

$$d^{3}q = q^{2} dq \sin \theta d\theta d\varphi = (k_{0} \sin \theta_{c} + q'_{\rho}) dq'_{\rho} dq'_{z} d\varphi.$$
(47)

In a neighborhood of the decay threshold $k = k_{\rm C}$ (where $E_{\rm ext} \rightarrow 2\Delta^{\rm RPA}$), the integrand in (40) has a pole at the point $[q = k_0, \theta = \theta_c]$. We have $|q'_z| \ll k_0$ and $|q'_{\rho}| \ll k_0$ in a neighborhood of the singularity as $q \rightarrow k_0, \theta \rightarrow \theta_c$. Then we can write the following expansions near the singularity:

$$d^3q \approx k_0 \sin \theta_c dq'_\rho dq'_z d\varphi,$$

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$$q \approx k_0 + q_z' \cos \theta_c + q_\rho' \sin \theta_c,$$

$$|\mathbf{k} - \mathbf{q}| \approx k_0 + q'_{\rho} \sin \theta_c - q'_z \cos \theta_c,$$

 $\mathbf{kq} \approx kk_0 \cos \theta_c + O(q'_{\rho}, q'_z),$

$$(\mathbf{k} - \mathbf{q})\mathbf{q} \approx k_0^2 \cos 2\theta_c + O(q'_{\rho}, q'_z).$$
(48)

In the limit $q \to k_0$, the energies of products of the decay have a view:

$$E_{\text{ext}}^{\text{RPA}}(q) = \Delta^{\text{RPA}} + \frac{\hbar^2}{2\mu} (q'_z \cos\theta_c + q'_\rho \sin\theta_c)^2, \qquad (49)$$

$$E_{\rm ext}^{\rm RPA}(|\mathbf{k}-\mathbf{q}|) = \Delta^{\rm RPA} + \frac{\hbar^2}{2\mu} (q'_{\rho} \sin\theta_c - q'_z \cos\theta_c)^2.$$

Let's consider the spectrum of CE (40) in some neighborhood of the decay threshold $k \to k_{\rm C}$. Decomposing the integrand near the pole $q \to k_0$, $\theta \to \theta_c$ with the use of expansions (48) and (49), we have

$$-\frac{2}{N}\sum_{\mathbf{q}\neq 0}\frac{\varepsilon(\mathbf{k},\mathbf{q})\varepsilon(\mathbf{k}-\mathbf{q},\mathbf{q})S^{-1}(q)}{E_{\mathrm{ext}}^{\mathrm{RPA}}(|\mathbf{k}-\mathbf{q}|) + E_{\mathrm{ext}}^{\mathrm{RPA}}(q) - E_{\mathrm{ext}}(k)} \rightarrow$$
$$\rightarrow -\frac{2}{N}\frac{V}{(2\pi)^2}\left(\frac{\hbar^2k_0^2}{2m}\right)^2\frac{\mu}{\hbar^2}S^{-1}(k_0)\cos 2\theta_c\cos\theta_c\sin\theta_c\times$$
(50)

$$\times k \int \frac{dq'_z dq'_\rho}{\frac{\mu}{\hbar^2} (2\Delta^{\text{RPA}} - E_{\text{ext}}) + \left[(q'_\rho)^2 \sin^2 \theta_c + (q'_z)^2 \cos^2 \theta_c \right]}$$
(51)

However, integrals (50) and (51) are not equal, because the transition to the limit $q \to k_0$, $\theta \to \theta_c$ has been done in the integrand. The integration over the entire q-space results in the divergence. Then we must introduce some cut-off parameter ρ so as integral (51) is finite, on the one hand, and integrals (50) and (51) are approximately equal in a neighborhood of the point $q = k_0$: $k_0 - \rho < q < k_0 + \rho$, on the other hand.

Let's introduce the polar coordinates:

$$q_{\rho}'\sin\theta_c = \rho\cos\psi,$$

 $q_z'\cos\theta_c = \rho\sin\psi,$

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$$dq'_{\rho}dq'_{z} = \frac{\rho d\rho d\psi}{\cos\theta_{c}\sin\theta_{c}}.$$
(52)

Then integral (51) is reduced to the form

$$-\frac{2}{N}\frac{V}{2\pi}\varepsilon^2(k_0)\frac{\mu\cos 2\theta_c}{\hbar^2}S^{-1}(k_0)k\times$$

$$\times \int\limits_{0}^{\rho} \frac{\rho d\rho}{\frac{\hbar^2}{\mu} (2\Delta^{\rm RPA} - E_{\rm ext}) + \rho^2} =$$

$$= \frac{V}{N} \frac{\varepsilon^2(k_0)\mu\cos 2\theta_c}{2\pi\hbar^2 S(k_0)} k \ln\left[\frac{(2\Delta^{\rm RPA} - E_{\rm ext})\mu/\hbar^2}{(2\Delta^{\rm RPA} - E_{\rm ext})\mu/\hbar^2 + \rho^2}\right].$$
(53)

We can see that the final result depends on the unknown parameter ρ which determines the integration domain near the point $q = k_0$. Then ρ must satisfy the requirements:

1. The point $k_{\rm C}$ is the decay threshold: $E_{\rm ext}(k_{\rm C}) = 2\Delta^{\rm RPA}$.

2. In Fig. 1, we can see that the Feynman formula $E_{\text{ext}}^{\text{RPA}}(k) = \varepsilon(k)/S(k)$ in the limit $k \to 0$ gives a sound mode $c\hbar k$ with a correct sound velocity c. Hence, the total spectrum (40) must have the same asymptotics:

$$E_{\text{ext}}(k \to 0) = E_{\text{ext}}^{\text{RPA}}(k \to 0) = c\hbar k.$$
(54)

The second term of expression (40) in the limit $k \to k_{\rm C}$ is integral (51). We must join these two asymptotics in a single expression which is a sought dispersion curve. Hence, the parameter ρ is a function of the variable k: $\rho = \rho(k)$.

3. The parameter ρ must ensure the approximate equality of integrals (50) and (51) in a neighborhood of the point $q = k_0$. We have decomposed the integrand in (50) near the point $q = k_0$ in a series in ρ/k_0 :

$$q \approx k_0 + q'_z \cos \theta_c + q'_\rho \sin \theta_c \approx k_0 \left(1 + \rho/k_0\right),$$
$$|\mathbf{k} - \mathbf{q}| \approx k_0 + q'_\rho \sin \theta_c - q'_z \cos \theta_c \approx k_0 \left(1 + \rho/k_0\right),$$

$$k_0 \sin \theta_c + q'_{\rho} \approx k_0 \sin \theta_c \left(1 + \frac{\rho}{k_0 \sin \theta_c} \right) \Rightarrow$$
$$\Rightarrow \frac{\rho}{k_0 \sin \theta_c} \ll 1. \tag{55}$$

Hence, $\rho(k)$ must satisfy inequality (55).

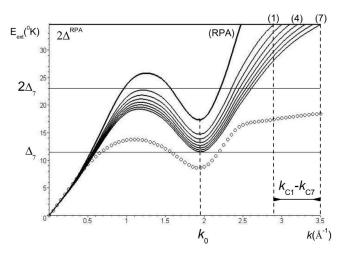


Fig. 3. Spectra of collective excitations. The line (RPA) is the spectrum corresponding to the Feynman formula (31). Lines 1-7 are dispersion curves obtained as the numerical solutions of Eq. (59) with parameters $k_{\rm C}$ equal to 2.9 Å⁻¹, 3.0 Å⁻¹, 3.1 Å⁻¹, 3.2 Å⁻¹, 3.3 Å⁻¹, 3.4 Å⁻¹, 3.5 Å⁻¹, respectively. The dotted line is the experimental spectrum of CE [28] at low temperatures. Dispersion curves 1–7 finish at the points $k = k_{\rm C}$ on the line $2\Delta^{\rm RPA}$

4. The spectrum of CE (40) must be determined with the parameter $\rho(k)$ by a self-consistent way.

In order to meet requirements (1-4), we must assume that

$$\frac{(2\Delta^{\text{RPA}} - E_{\text{ext}})\mu/\hbar^2}{(2\Delta^{\text{RPA}} - E_{\text{ext}})\mu/\hbar^2 + \rho^2} = \frac{2\chi\Delta^{\text{RPA}} - E_{\text{ext}}}{2\chi\Delta^{\text{RPA}}},$$
(56)

then

$$\rho^{2}(k) = \frac{\mu}{\hbar^{2}} \frac{E_{\text{ext}}(k) \left[2\Delta^{\text{RPA}} - E_{\text{ext}}(k) \right]}{2\chi \Delta^{\text{RPA}} - E_{\text{ext}}(k)},$$
(57)

where the parameter χ is determined by condition (44.1) $E_{\text{ext}}(k_{\text{C}}) = 2\Delta^{\text{RPA}}$:

$$\chi = \left[1 - \exp\left(\frac{2\Delta^{\text{RPA}} - E_{\text{ext}}^{\text{RPA}}(k_{\text{C}})}{\alpha k_{\text{C}}}\right)\right]^{-1}.$$
 (58)

As a result, the dispersion equation for CE (40) has a form

$$E_{\rm ext}(k) = E_{\rm ext}^{\rm RPA}(k) + \alpha k \ln\left[\frac{2\chi\Delta^{\rm RPA} - E_{\rm ext}(k)}{2\chi\Delta^{\rm RPA}}\right], \quad (59)$$

where

$$\alpha = \frac{V}{N} \frac{\varepsilon^2(k_0)\mu\cos 2\theta_c}{2\pi\hbar^2 S(k_0)}, \qquad \cos\theta_c = \frac{k_{\rm C}}{2k_0}.$$
 (60)

We can see that the parameter ρ is determined by the spectrum $E_{\text{ext}}(k)$. On the other hand, ρ determines this

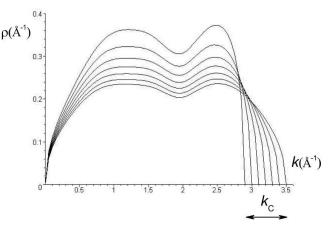


Fig. 4. Parameters of cut-off $\rho(k)$ for integral (53). The curves $\rho(k)$ correspond to the curves 1-7 in Fig. (3). A domain of the functions $\rho(k)$ is $0 \le k \le k_{\rm C}$

spectrum. $E_{\text{ext}}(k)$ doesn't contain ρ in an explicit form. Hence, $E_{\text{ext}}(k)$ is determined with the parameter ρ by a self-consistent way.

In the long-wave asymptotics, $E_{\text{ext}}^{\text{RPA}}(k \to 0) = c\hbar k + Ak^3$, A = const > 0. Then it is easily to show that

$$E_{\rm ext}(k \to 0) = c\hbar k - \frac{c\hbar\alpha}{2\chi\Delta^{\rm RPA}}k^2 + Ak^3 - \dots$$
 (61)

This means that the spectrum E_{ext} is joined with the Feynman formula at small k and describes the sound mode. Thus, condition (4.4.1) is satisfied. However, we can see that the even powers of k exist in expansion (61). But this doesn't contradict the isotropy of the liquid because the dispersion equation (59) depends on the modulus of the wave vector only: $E_{\text{ext}} = E_{\text{ext}}(|\mathbf{k}|)$.

We can see that the dispersion curve (59) depends on the parameter $k_{\rm C}$ (decay threshold) strongly. This is the *free parameter* being in the limits $k_{\rm C}^{\rm RPA} \leq k_{\rm C} \leq 2k_0$. Therefore, we have a family of curves shown in Fig. 3. The corresponding cut-off parameter ρ which joins the long-wave asymptotics $k \to 0$ with the asymptotics $k \to k_{\rm C}$ is shown in Fig. 4.

A domain of the function $\rho(k)$ is $0 \le k \le k_{\rm C}$ because, at $k > k_{\rm C}$, we have $\rho(k)^2 < 0$. This means that the dispersion curve (59) cannot be continued to the region $k > k_{\rm C}$ (though the function $E_{\rm ext}(k)$ exists formally). Hence, the point $k_{\rm C}$ is the end point of the spectrum. For the typical value $k_{\rm C} = 3.2$ Å⁻¹, we have: $\max(\rho/k_0) =$ $0.28/1.93 = 0.15 \ll 1$ and $\max(\rho/k_0/\sin\theta_c) = 0.27 < 1$. This means that condition (44.1) is satisfied.

The dispersion curves 1-7 in Fig. 3 are more close to the experimental curve than $E_{\text{ext}}^{\text{RPA}}(k)$. However, they have an essential defect. CE with the dispersion curve

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 $E_{\rm ext}(k)$ decays into excitations with the spectrum calculated in RPA: $E_{\rm ext}^{\rm RPA}(q)$ and $E_{\rm ext}^{\rm RPA}(|{\bf k}-{\bf q}|)$. This situation corresponds to the conservation of energy in the form (41). In reality, the law of conservation of energy is of the form (38), where the energy of decaying CE and the energies of decay products are determined with the real spectrum. We can see in Fig. 3 that the dispersion curve $E_{\rm ext}(k)$ differs from the curve $E_{\rm ext}^{\rm RPA}(k)$ essentially in the region of big k. So, the new value of a roton gap is $\Delta < \Delta^{\rm RPA}$. This means that the energy is not conserved at the decay of CE into two rotons. In other words, the dispersion curve $E_{\rm ext}(k)$ is not self-consistent.

4.2. The self-consistent form of the dispersion curve $E_{\text{ext}}(k)$

The dispersion equation $E_{\text{ext}}(k)$ is self-consistent if the energy of the end point of the spectrum is equal to the doubled roton gap of this spectrum: $E_{\text{ext}}(k_{\text{C}}) = 2\Delta$. Let the new spectrum have the form

$$E_{\text{ext}}(k) = E_{\text{ext}}^{\text{RPA}}(k) + \alpha k \ln\left[\frac{2\widetilde{\Delta} - E_{\text{ext}}(k)}{2\widetilde{\Delta}}\right], \quad (62)$$

where the parameter $\tilde{\Delta}$ must be such that the condition of self-consistency is executed:

$$\left\{\begin{array}{l}
E_{\text{ext}}(k_{\text{C}}) = 2\Delta \\
E_{\text{ext}}(k_0) = \Delta
\end{array}\right\}.$$
(63)

The parameter Δ is the *new* roton gap at the point k_0 . Then the system of equations (63) in the expanded form is

$$\left\{ \begin{array}{l} 2\Delta = E_{\text{ext}}^{\text{RPA}}(k_{\text{C}}) + \alpha k_{\text{C}} \ln \left(1 + \frac{\Delta}{\tilde{\Delta}}\right) \\ \Delta = E_{\text{ext}}^{\text{RPA}}(k_{0}) + \alpha k_{0} \ln \left(1 + \frac{\Delta}{2\tilde{\Delta}}\right) \end{array} \right\}.$$
(64)

The system of equations (62) and (64) determines a dispersion curve of CE. The results of numerical solution of these equations with $k_{\rm C} = 2.9 \text{ Å}^{-1} - 3.5 \text{ Å}^{-1}$ are shown in Fig. 5. Curves 1-7 in Fig. 5 correspond to curves 1-7in Fig. 4. As in the previous case, the spectrum depends on its end point $k_{\rm C}$ strongly though the sound velocity $\hbar c = \lim_{k \to 0} \frac{\partial E_{\text{ext}}}{\partial k}$ is the same in the all cases. We can see a weak pinning of the curve $E_{\text{ext}}(k)$ to the line 2Δ . This means the hybridization of the dispersion curve of CE with a two-roton level [27]. On the rest of regions, the energy $E_{\text{ext}}(k)$ is determined by a state with one CE (phonon or roton) completely. We have the family of curves E_{ext} , and we cannot obtain the point k_{C} on this step of calculations. In order to do this, we must generalize the oscillator model formulated in Subsection 33.2.

ISSN 2071-0194. Ukr. J. Phys. 2011. Vol. 56, No. 11

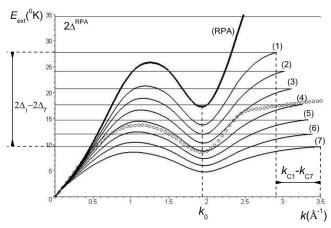


Fig. 5. Spectra of collective excitations. The line (RPA) is the spectrum corresponding to the Feynman formula (31). Lines 1–7 are dispersion curves obtained by the numerical solution of the system of equations (62) and (64) with parameters $k_{\rm C} = 2.9$ Å⁻¹, 3.0 Å⁻¹, 3.1 Å⁻¹, 3.2 Å⁻¹, 3.3 Å⁻¹, 3.4 Å⁻¹, 3.5 Å⁻¹, respectively. The dotted line is the experimental spectrum of CE [28]. The dispersion curves 1–7 are ended at the points $k = k_{\rm C}$ on the lines $2\Delta_{1-7}$

5. The Ground State and Bose Condensate

5.1. Formalism of effective mass in the oscillator model

In this section, our problem is the calculation of the ground-state energy taking the anharmonic correction in Eq. (15) into consideration. If we calculate this correction, then we have a divergence $E_0 = E_0^{\text{RPA}} + \infty$ as in Section 4. In order to overcome this difficulty, let's use the oscillator model formulated in Section 3, where the superfluid liquid is a totality of independent harmonic oscillators with frequencies $E_{\text{ext}}^{\text{RPA}}(k) = \varepsilon(k)/S(k)$. In higher approximations, we have another spectra of CE $E_{\text{ext}}(k)$: the system of equations (62) and (64). However, this spectrum can be written by analogy with RPA as

$$E_{\text{ext}}(k) = \frac{\tilde{\varepsilon}(k)}{S(k)}, \quad \text{where} \quad \tilde{\varepsilon}(k) = \frac{\hbar^2 k^2}{2\tilde{m}(k)}.$$
 (65)

Due to the contribution of anharmonic terms of Hamiltonian (10), the mass of a *particle* m is renormalized to mass of a *quasiparticle* $\tilde{m}(k)$. Continuing the analogy with RPA, we can write the effective Hamiltonian having a form as in RPA:

$$\hat{H}_{\text{eff}} = \sum_{\mathbf{k}_1 \neq 0} \tilde{\varepsilon}(k_1) \left(-\frac{\partial^2}{\partial \rho_{\mathbf{k}_1} \partial \rho_{-\mathbf{k}_1}} + \frac{1}{4} \rho_{\mathbf{k}_1} \rho_{-\mathbf{k}_1} - \frac{1}{2} \right) + \frac{N^2}{2V} \tilde{\nu}(0) + \frac{N}{2V} \sum_{\mathbf{k}_1 \neq 0} \tilde{\nu}(k_1) \left(\rho_{\mathbf{k}_1} \rho_{-\mathbf{k}_1} - 1 \right)$$
(66)

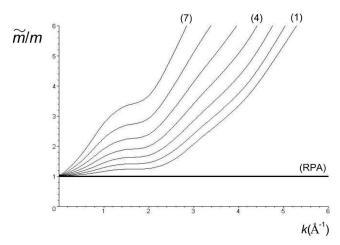


Fig. 6. Effective masses of quasiparticles in units of the mass of ⁴He: \tilde{m}/m . The curve (RPA) corresponds to a "naked" particle. The numbers 1–7 correspond to curves in Fig. 5. The functions $\tilde{m}(k)$ have a sense in the range $k < k_{\rm C}$ only

and the corresponding Jacobian:

$$\ln J = \ln \left(V^N \prod_{\mathbf{k}\neq 0}' \frac{1}{\pi} \right) - \frac{1}{2} \sum_{\mathbf{k}\neq 0} \rho_{\mathbf{k}} \rho_{-\mathbf{k}}, \tag{67}$$

where the normalization requirement (5) has been used.

We must obtain the same structure factor S(k) in any approximation, because this function is given by experiment. Therefore, we must introduce the effective interaction $\tilde{\nu}(k)$ as follows:

$$S(k) = -\frac{1}{4f(k)} = \frac{1}{\sqrt{1 + \frac{2N}{V}\frac{\nu(k)}{\varepsilon(k)}}} = \frac{1}{\sqrt{1 + \frac{2N}{V}\frac{\widetilde{\nu}(k)}{\widetilde{\varepsilon}(k)}}} \Rightarrow$$
$$\Rightarrow \widetilde{\nu}(k) = \widetilde{\varepsilon}(k)\frac{V}{2N}\left[\frac{1}{S(k)^2} - 1\right]. \tag{68}$$

The effective masses and interactions are shown in Figs. 6 and 7. It is necessary to note that $\tilde{m}(k \to 0) = m$ and $\tilde{\nu}(0) = \nu(0)$.

As a result, we have the totality of harmonic oscillators again. These oscillators have the same dispersions $\langle \rho_{\mathbf{k}} \rho_{-\mathbf{k}} \rangle$ as in RPA. However, they have another frequencies $E_{\text{ext}}(k)$ instead of the old ones $E_{\text{ext}}^{\text{RPA}}(k)$. The difference between the new frequencies and the initial frequencies depends on the aforesaid anharmonicities. The equation of motion for each oscillator can be written as Eq. (32) but with an effective mass and an effective interaction:

$$-\frac{\hbar^2}{2\widetilde{M}(k)}\frac{\partial^2\bar{\psi}}{\partial\rho_{\mathbf{k}}\partial\rho_{-\mathbf{k}}}+$$

$$+\left[\frac{1}{4}\widetilde{\varepsilon}(k) + \frac{N}{2V}\widetilde{\nu}(k)\right]\rho_{\mathbf{k}}\rho_{-\mathbf{k}}\bar{\psi} = \widetilde{\xi}(k)\bar{\psi}.$$
(69)

The ground-state energy can be rewritten as follows:

$$E_{0} = \sum_{\mathbf{k}\neq 0} \frac{1}{2} \frac{\widetilde{\varepsilon}(k)}{S(k)} - \sum_{\mathbf{k}\neq 0} \left[\frac{1}{2} \widetilde{\varepsilon}(k) + \frac{N}{2V} \widetilde{\nu}(k) \right] + \frac{N^{2}}{2V} \widetilde{\nu}(0).$$
(70)

It is worth noting that we must do the transition from the summation over \mathbf{k} to the integration as follows:

$$\sum_{\mathbf{k}\neq 0} \to \frac{V}{(2\pi)^3} \int_0^{k_{\rm C}} k^2 dk.$$
(71)

The results of calculations of the ground-state energy (per atom) for particles' system (RPA) and for quasiparticles' system (curves 1-7) are:

$$E_0^{\text{RPA}}/N = -13.78 \text{ K}, \qquad E_0^{(1)}/N = -8.73 \text{ K},$$

 $E_0^{(2)}/N = -6.66 \text{ K}, \qquad E_0^{(3)}/N = -4.62 \text{ K},$
 $E_0^{(4)}/N = -2.60 \text{ K}, \qquad E_0^{(5)}/N = -0.59 \text{ K},$
 $E_0^{(6)}/N = 1.43 \text{ K} \qquad E_0^{(7)}/N = 3.43 \text{ K}.$ (72)

We can see that the existence of the end point of a dispersion curve causes some increase of the ground-state energy. Since $k_{\rm C}$ is unknown, we cannot select a value of this energy. The energy E_0 is minimal at $k_{\rm C} < 2.9$ Å⁻¹. But the important condition for oscillator frequencies $\hbar\omega = E_{\rm ext}$ exists still.

If the velocity of a CE $\frac{\partial E_{\text{ext}}}{\partial p} \equiv \frac{\partial \hbar \omega}{\partial p}$ is more than the sound velocity in a system, then CE radiates a phonon [26]. The regions of a dispersion curve, where such event is possible, is unstable. We have formulated the oscillator model of Bose liquid, where its ground-state energy is a sum of the energies of ground states of oscillators representing the liquid. In other words, the ground state is an infinity number of *virtual* collective excitations. Then *in order to determine the ground state as a state with minimal energy, the dispersion curve* $E_{\text{ext}}(k)$ *must be stable.* It means that, for all k, the following inequality must be executed:

$$\frac{\partial E_{\text{ext}}(k)}{\partial k} \equiv <\lim_{k \to 0} \frac{\partial E_{\text{ext}}(k)}{\partial k} = c\hbar.$$
(73)

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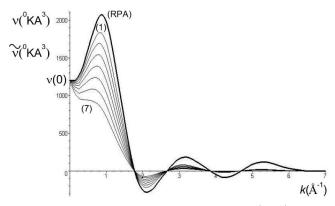


Fig. 7. Potential of interaction between particles (RPA) and between quasiparticles $(1\mathcar{-}7)$

If this condition is not satisfied, then the ground state falls apart. The plots of CE's velocity are shown in Fig. 8. Curves 4-7 satisfy criterion (73). Hence, the possible end points are present in the interval $k_{\rm C} = 3.2 \text{ Å}^{-1} \div 2k_0$ only. Spectrum 4 corresponds to the minimal value $k_{\rm C} =$ 3.2 Å^{-1} . On the contrary, the curve (RPA) is unstable almost completely.

We can see in (72) that an increase of $k_{\rm C}$ causes an increase of E_0 : $E_0^{(4)} < E_0^{(5)} < E_0^{(6)} < E_0^{(7)}$. Hence, the energy $E_0^{(4)}$ is minimal for all allowed energies E_0 . This means that

$$E_0/N = E_0^{(4)}/N = -2.60 \text{ K.}$$
 (74)

The experimental value is $E_0/N = -7.12$ K. It is necessary to note that the short-range correlations make essential contributions to E_0 . These correlations are calculated badly within the method of collective variables. So, a hybrid approach was proposed in [22], where the transition to collective variables was made not completely, and a part of the coordinates was kept as Cartesian coordinates. Proceeding from the aforesaid, we can consider result (74) as satisfactory.

The final spectrum of a collective excitation $E_{\text{ext}}(k)$ is shown in Fig. 9. The dispersion curve has been obtained as a numerical solution of the system of equations (62) and (64) with the optimal parameter $k_{\text{C}} = 3.2 \text{ Å}^{-1}$. We can see a weak pinning of the dispersion curve to the line 2Δ , which means the decay of CE into two rotons with energy Δ and momentum k_0 in each. The dispersion curve coincides with the experimental curve well.

5.2. Suppression of Bose condensate

In a Bose system at sufficiently low temperatures, the occupation number N_0 of the state with minimal energy (momentum of particles is $\mathbf{p} = 0$) is a macroscopic

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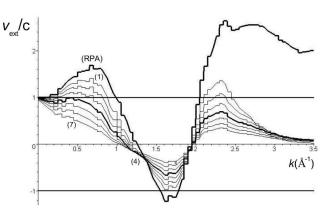


Fig. 8. Velocities of collective excitations $v_{\text{ext}}(k) = \frac{\partial E_{\text{ext}}(k)}{\hbar \partial k}$ in units of a sound velocity $c. v_{\text{ext}}(k) < 0$ means that the velocity and the momentum **k** have contrary directions. The curve (RPA) corresponds to the Feynman spectrum. Curves 1-7 correspond to the curves in Fig. 5. Condition (73) is satisfied for the curves where $|v_{\text{ext}}(k)|/c < 1$ for all k. Spectra 4-7 are stable at the radiation of a phonon. Spectrum 4 (with $k_{\text{C}} = 3.2$ Å⁻¹, it is marked by a bold line) is on the limit of stability

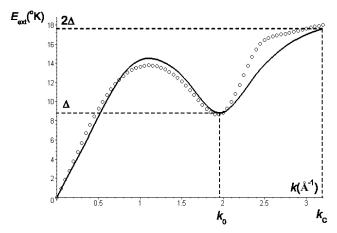


Fig. 9. Dispersion curve of CE obtained with the optimal parameter $k_{\rm C} = 3.2$ Å⁻¹. As a result, we have: $\mu = 0.19~m$ (the new roton mass), Δ =8.8 K, $k_0 = 1.95$ Å⁻¹. The dotted line is the experimental spectrum of CE [28] at low temperatures. At the point $k = k_{\rm C}$ on the line 2 Δ , the dispersion curve ends

number $N_0 \leq N$. For the ideal gas, the density of a condensate and the temperature of the transition are

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_0}\right)^{3/2}, \qquad T_0 = \frac{2\pi\hbar^2}{m} \left(\frac{N/V}{2.612}\right)^{2/3}.$$
 (75)

At the temperature T = 0, all atoms are in BC: $N_0 = N$. If the particles interact, then BC is suppressed. BC is suppressed strongly in He II: $N_0/N = 0.07$. In paper [3], the model was proposed where BC is suppressed due to the formation of pairs of bosons. In this section, we will consider the suppression of BC from the standpoint

of collective motions of the liquid using the oscillator model.

Equations (32) or (69) describe harmonic oscillations of the Bose liquid. According to the uncertainty principle, the energy of an oscillator in the ground state cannot be zero, $1/2\hbar\omega \neq 0$. The energy is divisible into the kinetic energy and the potential energy in equal parts $\langle T \rangle = \langle U \rangle = M\omega^2 \langle \rho_{\bf k} \rho_{-\bf k} \rangle/2 = \xi/2$ according to the virial theorem. This zero-point energy is the energy of fluctuations of the quantum liquid. Hence, collective motions are in the ground state, and no all particles can be in BC. In other words, BC is suppressed by dynamical fluctuations [29].

Using Eq. (24), we write the energy of the ground state in the form

$$\sum_{\mathbf{k}\neq 0} \varepsilon(k) \left[-4f^2(k)\rho_{\mathbf{k}}\rho_{-\mathbf{k}} - 2f(k) + \frac{1}{4}\rho_{\mathbf{k}}\rho_{-\mathbf{k}} - \frac{1}{2} \right] +$$

$$+\frac{N^2}{2V}\nu_0 + \sum_{\mathbf{k}\neq 0} \frac{N}{2V}\nu_k(\rho_{\mathbf{k}}\rho_{-\mathbf{k}} - 1) = E_0.$$
(76)

After the averaging of this expression according to the rule $\rho_{\mathbf{k}}\rho_{-\mathbf{k}} \rightarrow \langle \rho_{\mathbf{k}}\rho_{-\mathbf{k}} \rangle$, in view of the expression for the potential energy of the system

$$\sum_{1 \le i < j \le N} \Phi(|\mathbf{r}_i - \mathbf{r}_j|) = \frac{N^2}{2V} \nu_0 + \sum_{\mathbf{k} \ne 0} \frac{N}{2V} \nu_k (\langle \rho_{\mathbf{k}} \rho_{-\mathbf{k}} \rangle - 1)$$
(77)

and the evident equality $E_0 = \langle T \rangle + \langle \Phi \rangle$, we can write the average kinetic energy of the system as

$$\langle T \rangle = \sum_{\mathbf{k} \neq 0} \varepsilon(k) \left[\left(-4f^2(k) + \frac{1}{4} \right) \langle \rho_{\mathbf{k}} \rho_{-\mathbf{k}} \rangle - 2f(k) - \frac{1}{2} \right].$$
(78)

Since $\varepsilon(k)$ is the kinetic energy of a particle, the expression in the square brackets can be understood as the occupation numbers of above-condensate particles $N_{\mathbf{k}\neq 0}$. Using connection (29), we can write the kinetic energy and the corresponding occupation number via the function f(k) or via the structure factor S(k):

$$\langle T \rangle = \sum_{\mathbf{k} \neq 0} \frac{\hbar^2 k^2}{2m} \left[\frac{(4f(k) + 1)^2}{-16f(k)} \right],\tag{79}$$

$$N_{\mathbf{k}\neq 0} = \frac{(4f(k)+1)^2}{-16f(k)} = \frac{(S(k)-1)^2}{4S(k)}.$$
(80)

Then the density of BC is

$$N_0 = N - \sum_{\mathbf{k} \neq 0} N_{\mathbf{k}} = N - \frac{V}{(2\pi)^3} \int_0^\infty \frac{(S-1)^2}{4S} 4\pi k^2 dk.$$
(81)

In the case of non-interacting particles, we have f(k) = -1/4 and S(k) = 1; hence, $N_{\mathbf{k}} = 0$, $N_0 = N$. In the case of a weakly non-ideal gas with the interaction $\nu_{\mathbf{k}} = \frac{4\pi\hbar^2}{m}a$ and the scattering length $\frac{a^3}{V/N} \ll 1$, the density of BC is

$$\frac{N_0}{N} = 1 - \frac{8}{3}\sqrt{\frac{Na^3}{\pi V}}$$
(82)

that coincides with the result of Bogolyubov [26].

The expression for the density of BC (81) is correct for systems with weak interaction only. As it has been shown in [20, 21], in the general case, we must use the expression

$$\frac{N_0}{N} = F(R \to \infty) = \exp\left(-\frac{V}{(2\pi)^3 N} \int_0^\infty N_\mathbf{k} 4\pi k^2 dk\right),\tag{83}$$

where $F(\mathbf{r}|\mathbf{r}')$ is the one-particle density matrix, and $R = |\mathbf{r}' - \mathbf{r}|$. Expression (81) is the two first terms of the expansion of exponent (83). In RPA, the density of BC is

$$\left(\frac{N_0}{N}\right)_{\rm RPA} = 0.263. \tag{84}$$

In the higher approximations, we have the effective Hamiltonian (66). In order to calculate the density of BC with the effective Hamiltonian $\hat{H}_{\rm eff}$ (66), we are going to proceed from the following reason. Let's write the ground-state energy of the Bose system in the form

$$\sum_{\mathbf{k}\neq 0} \widetilde{\varepsilon}(k) \left[\frac{(S(k)-1)^2}{4S(k)} \right] + \frac{N^2}{2V} \nu_0 + \sum_{\mathbf{k}\neq 0} \frac{N}{2V} \widetilde{\nu}_k[S(k)-1] = E_0.$$
(85)

We must mark out the kinetic energy of the system of *particles*. All anharmonic terms in the Hamiltonian $\widehat{H}(10)$ or in the Hamiltonian \widehat{H}_{BZ} (6) are the terms of a operator of kinetic energy $\sum_{1 \leq j \leq N} \frac{\hat{p}_j^2}{2m}$. This means that the renormalization of mass $m \to \widetilde{m}$ and interaction $\nu(k) \to \widetilde{\nu}(k)$ occurs due to the contribution of the

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kinetic energy, but not the interaction as in usual perturbation theory. Hence, the potential energy of the system $\sum_{1 \leq i < j \leq N} \Phi(|\mathbf{r}_i - \mathbf{r}_j|)$ (77) is invariable at the transition from \hat{H} to \hat{H}_{eff} . In order to obtain the new kinetic energy of particles, let's rewrite (85) in the identical form:

$$\sum_{\mathbf{k}\neq 0} \left(\widetilde{\varepsilon}(k) \left[\frac{(S(k)-1)^2}{4S(k)} \right] + \frac{N}{2V} (\widetilde{\nu}_k - \nu_k) [S(k)-1] \right) +$$

$$+\frac{N^2}{2V}\nu_0 + \sum_{\mathbf{k}\neq 0} \frac{N}{2V}\nu_k[S(k) - 1] = E_0.$$
(86)

Proceeding from the aforesaid, the first term is a new kinetic energy of particles. In order to obtain the momentum distribution $N_{\mathbf{k}}$ of particles, let's mark out the kinetic energy of a *particle* $\varepsilon(k)$ in this expression. Then we have

$$\langle T \rangle = \sum_{\mathbf{k} \neq 0} \varepsilon(k) \left(\frac{\widetilde{\varepsilon}(k)}{\varepsilon(k)} \left[\frac{(S(k) - 1)^2}{4S(k)} \right] + \frac{N}{2V} \frac{\widetilde{\nu}_k - \nu_k}{\varepsilon(k)} [S(k) - 1] \right),$$

$$(87)$$

$$N_{\mathbf{k}\neq 0} = \frac{\widetilde{\varepsilon}(k)}{\varepsilon(k)} \left[\frac{(S(k)-1)^2}{4S(k)} \right] + \frac{N}{2V} \frac{\widetilde{\nu}_k - \nu_k}{\varepsilon(k)} [S(k)-1].$$
(88)

Substituting (88) in (83), we obtain the densities of BC for the dispersion curves 1-7 in Fig. 5:

$$N_0^{(1)}/N = 0.149,$$
 $N_0^{(2)}/N = 0.104,$
 $N_0^{(3)}/N = 0.071,$ $N_0^{(4)}/N = 0.048,$
 $N_0^{(5)}/N = 0.031,$ $N_0^{(6)}/N = 0.020,$

 $N_0^{(7)}/N = 0.013. (89)$

As has been written above, curve 4 with $k_{\rm C} = 3.2 \text{ Å}^{-1}$ is realized in practice only. This means that the portion of BC in superfluid helium at zeroth temperature is $N_0/N = 0.048$. The density of BC measured in experiment by the method of deep inelastic scattering of neutrons [30] and by the method of quantum evaporation [31] is 0.07. Hence, result (89) is satisfactory fully.

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6. Conclusion

As a result of the self-consistent solution of the Schrödinger equation for the state of the Bose liquid with one CE, the dispersion law $E_{ext}(k)$ (the system of equations (62) and (64)) has been obtained. It has been shown that, for the Hermitian form of the Bogolyubov–Zubarev Hamiltonian, the second term in the Bijl–Dingle–Jastrow expansion considers the real and virtual processes of decay of CE. Higher terms in this expansion consider the decays into three and more excitations, which are very improbable processes. The decay of CE on two rotons causes the existence of the end point $k_{\rm C}$ of a dispersion curve. Our main result is: the phonon-roton dispersion curve $E_{\text{ext}}(k)$ is determined by both the interaction between bosons $\nu(k)$ and the end point $k_{\rm C}$. That is, the dispersion curve strongly depends on the property of its stability.

In order to find $k_{\rm C}$ and the ground-state energy, we have been formulated the oscillator model of Bose liquid. According to this model, the basic Bogolyubov-Zubarev Hamiltonian can be rewritten as a Hamiltonian in the harmonic approximation with renormalized kinetic and potential energies. As a result, we have a totality of harmonic oscillators again with the same dispersions S(k) but with another frequencies already. The ground-state energy E_0 depends on these frequencies; hence, it depends on the end point $k_{\rm C}$. Proceeding from the condition of minimum of the energy and from the condition of stability of the ground state, we can obtain the unknown end point $k_{\rm C}=3.2$ Å⁻¹ of the spectrum. The obtained spectrum of CE, E_{ext} , is a function connecting the energy of an excitation with the structure factor S(k) of the liquid which is taken from the experiment. Thus, we did not use any model potentials of interaction. This means that all our calculations have been done without any adaption parameters.

A mechanism of suppression of one-particle BC has been described at the temperature of absolute zero. As a consequence of the uncertainty principle, the dynamical fluctuations exist in the ground state and give a nonzero kinetic energy. These fluctuations suppresses BC. It has been shown that such fluctuations are absent for the ideal gas. It is necessary to note that the analogous dynamical quantum fluctuations in other systems can cause quantum phase transitions [32]. At nonzero temperatures, BC is suppressed by both dynamical fluctuations and kinematic (thermal) fluctuations.

APPENDIX

A. The Operator of Momentum

Let's consider the expression

$$J^{1/2} \hat{\mathbf{P}} J^{-1/2} \bar{\psi} = -\sum_{\mathbf{k}_{1} \neq 0} \hbar \mathbf{k}_{1} \rho_{\mathbf{k}_{1}} J^{1/2} \frac{\partial}{\partial \rho_{\mathbf{k}_{1}}} \left[J^{-1/2} \bar{\psi} \right] =$$

$$= \frac{1}{2} \sum_{\mathbf{k}_{1} \neq 0} \hbar \mathbf{k}_{1} \rho_{\mathbf{k}_{1}} \frac{\partial \ln J}{\partial \rho_{\mathbf{k}_{1}}} + \hat{\mathbf{P}} \bar{\psi} =$$

$$= \frac{1}{2} \sum_{\mathbf{k} \neq 0} \sum_{\mathbf{k}_{1} \neq 0} \hbar \mathbf{k}_{1} \rho_{\mathbf{k}_{1}} \frac{\partial}{\partial \rho_{\mathbf{k}_{1}}} \left[\ln C - \frac{1}{2} \rho_{\mathbf{k}} \rho_{-\mathbf{k}} \right] +$$

$$+ \frac{1}{2} \sum_{\mathbf{k} \neq 0} \sum_{\mathbf{q} \neq 0} \sum_{\mathbf{k}_{1} \neq 0} \hbar \mathbf{k}_{1} \rho_{\mathbf{k}_{1}} \frac{\partial}{\partial \rho_{\mathbf{k}_{1}}} \left[\frac{1}{6} \rho_{\mathbf{k}} \rho_{\mathbf{q}-\mathbf{k}} \rho_{-\mathbf{q}} \right] +$$

$$+ \dots + \hat{\mathbf{P}} \bar{\psi} = -\frac{1}{2} \sum_{\mathbf{k} \neq 0} [\hbar \mathbf{k} \rho_{\mathbf{k}} \rho_{\mathbf{q}-\mathbf{k}} - \hbar \mathbf{k} \rho_{\mathbf{k}} \rho_{-\mathbf{k}}] +$$

$$+ \frac{1}{6} \sum_{\mathbf{k} \neq 0} \sum_{\mathbf{q} \neq 0} [\hbar \mathbf{k} \rho_{\mathbf{k}} \rho_{\mathbf{q}-\mathbf{k}} \rho_{-\mathbf{q}} +$$

$$+ \hbar (\mathbf{q} - \mathbf{k}) \rho_{\mathbf{k}} \rho_{\mathbf{q}-\mathbf{k}} \rho_{-\mathbf{q}} + \hbar (-\mathbf{q}) \rho_{\mathbf{k}} \rho_{\mathbf{q}-\mathbf{k}} \rho_{-\mathbf{q}}] -$$

$$- \dots + \hat{\mathbf{P}} \bar{\psi} = 0 + \hat{\mathbf{P}} \bar{\psi} \Longrightarrow \hat{\mathbf{P}} \bar{\psi} = \mathbf{P} \bar{\psi}. \tag{A1}$$

That is, if the function ψ is an eigenfunction of the operator of momentum $\hat{\mathbf{P}}$, then $\bar{\psi}$ is an eigenfunction of the operator of momentum too.

B. The Wave Function of a System of Free Bosons

If we exclude the interaction between particles, $\nu(k) = 0$, the wave function of a system $\psi = \bar{\psi} J^{-1/2}$ must be a wave function of free bosons. So, we can write for the ground state:

$$\psi = Be^U J^{-1/2} = \text{const} \Rightarrow U = \frac{1}{2} \ln J, \tag{B1}$$

where B is a normalization constant. Let's verify it. In the ground state of a system of noninteracting bosons, $E_0 = 0$. Then, proceeding from Eq. (15), we can write

$$-\frac{\partial^{2}U}{\partial\rho_{\mathbf{k}_{1}}\partial\rho_{-\mathbf{k}_{1}}} - \frac{\partial U}{\partial\rho_{\mathbf{k}_{1}}}\frac{\partial U}{\partial\rho_{-\mathbf{k}_{1}}} - \frac{1}{4}\rho_{\mathbf{k}_{1}}\frac{\partial\ln J}{\partial\rho_{\mathbf{k}_{1}}} - \frac{1}{2} + \sum_{\mathbf{k}_{2}\neq0}\frac{\mathbf{k}_{1}\cdot\mathbf{k}_{2}}{k_{1}^{2}\sqrt{N}}\rho_{\mathbf{k}_{1}+\mathbf{k}_{2}}\left[\frac{\partial U}{\partial\rho_{\mathbf{k}_{1}}\partial\rho_{\mathbf{k}_{2}}} + \frac{\partial U}{\partial\rho_{\mathbf{k}_{1}}}\frac{\partial U}{\partial\rho_{\mathbf{k}_{2}}}\right] = 0.$$
(B2)

Now let's rewrite the third term of Eq. (B2) in the form

$$-\frac{1}{4}\frac{\partial \ln J}{\partial \rho_{\mathbf{k}_{1}}} \left[-\frac{\partial \ln J}{\partial \rho_{-\mathbf{k}_{1}}} + \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\neq 0} \frac{\mathbf{k}\mathbf{k}'}{k^{2}} \rho_{\mathbf{k}+\mathbf{k}'} \frac{\partial \ln J}{\partial \rho_{\mathbf{k}'}} \right] = \\ = \frac{\partial U}{\partial \rho_{\mathbf{k}_{1}}} \frac{\partial U}{\partial \rho_{-\mathbf{k}_{1}}} - \sum_{\mathbf{k}_{2}\neq 0} \frac{\mathbf{k}_{1} \cdot \mathbf{k}_{2}}{k_{1}^{2}\sqrt{N}} \rho_{\mathbf{k}_{1}+\mathbf{k}_{2}} \frac{\partial U}{\partial \rho_{\mathbf{k}_{1}}} \frac{\partial U}{\partial \rho_{\mathbf{k}_{2}}}, \tag{B3}$$

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where we used Eq. (11) for the Jacobian and equality (B1). After that, we have the equation

$$-\frac{\partial^2 U}{\partial \rho_{\mathbf{k}_1} \partial \rho_{-\mathbf{k}_1}} - \frac{1}{2} + \sum_{\mathbf{k}_2 \neq 0} \frac{\mathbf{k}_1 \cdot \mathbf{k}_2}{k_1^2 \sqrt{N}} \rho_{\mathbf{k}_1 + \mathbf{k}_2} \frac{\partial U}{\partial \rho_{\mathbf{k}_1} \partial \rho_{\mathbf{k}_2}} = 0.$$
(B4)

With the help of relation (B1), we can write

$$-\frac{1}{2}\frac{\partial}{\partial\rho_{\mathbf{k}_{1}}}\left[\rho_{\mathbf{k}_{1}}+\frac{\partial\ln J}{\partial\rho_{-\mathbf{k}_{1}}}-\frac{1}{\sqrt{N}}\sum_{\mathbf{k}_{1}\neq0}\frac{\mathbf{k}_{1}\mathbf{k}_{2}}{k_{1}^{2}}\rho_{\mathbf{k}_{1}+\mathbf{k}_{2}}\frac{\partial\ln J}{\partial\rho_{\mathbf{k}_{2}}}\right]=0,\quad(B5)$$

because the expression in the square brackets coincides with Eq. (11). We can see that the wave function (B1) satisfies the Schrödinger equation (15).

Let's obtain the normalization constant B. Let the wave function of the ground state $\bar{\psi}$ (23) be determined by the following way in RPA:

$$\bar{\psi} = A \exp\left[-\frac{1}{4} \sum_{\mathbf{k} \neq 0} \frac{1}{S(k)} \rho_{\mathbf{k}} \rho_{-\mathbf{k}}\right],\tag{B6}$$

where (29) was taken into account. The constant A is obtained from the normalization condition (7) in the thermodynamical limit $N \to \infty$:

$$\prod_{\mathbf{k}\neq 0}^{\prime} \int_{-\infty}^{\infty} d\rho_{\mathbf{k}}^{c} \int_{-\infty}^{\infty} d\rho_{\mathbf{k}}^{c} |\bar{\psi}|^{2} = 1 \Rightarrow A = \prod_{\mathbf{k}\neq 0}^{\prime} \sqrt{\frac{1}{\pi S(k)}}.$$
 (B7)

Let's write the Jacobian in RPA as

$$J = C \exp\left[-2\sum_{k\neq 0}^{\prime} (\rho_{k}^{c})^{2} + (\rho_{k}^{s})^{2}\right].$$
 (B8)

The constant C is obtained from condition (5) in the thermodynamical limit $N \to \infty$:

$$V^{N} = \prod_{\mathbf{k}\neq 0}^{\prime} \int_{-\infty}^{\infty} d\rho_{\mathbf{k}}^{c} \int_{-\infty}^{\infty} d\rho_{\mathbf{k}}^{c} J \Rightarrow C = V^{N} \prod_{\mathbf{k}\neq 0}^{\prime} \frac{1}{\pi}.$$
 (B9)

Then

$$\psi = J^{-1/2} \bar{\psi} = \frac{1}{\sqrt{V^N}} \prod_{\mathbf{k} \neq 0} \frac{1}{\sqrt{S(k)}} \times \\ \times \exp\left(-\frac{1}{4} \sum_{\mathbf{k} \neq 0} \left[\frac{1}{S(k)} - 1\right] \rho_{\mathbf{k}} \rho_{-\mathbf{k}}\right).$$
(B10)

If the interaction between particles is absent, then S(k) = 1, and the wave function of the system ψ transforms to the wave function of a system of free bosons $\psi_{\nu=0} = 1/\sqrt{V^N}$, and the normalization constant is

$$B = 1/\sqrt{V^N}.$$
(B11)

The constant B is the same for higher powers of the expansions of the wave function and the Jacobian.

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Received 01.10.10

САМОУЗГОДЖЕНА МІКРОСКОПІЧНА МОДЕЛЬ ЕНЕРГЕТИЧНОГО СПЕКТРА НАДПЛИННОГО ⁴Не НА ЕРМІТОВІЙ ФОРМІ ГАМІЛЬТОНІАНА БОГОЛЮБОВА–ЗУБАРЄВА

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Резюме

Ґрунтуючись на представленні колективних змінних з ермітовою формою гамільтоніана Боголюбова–Зубарєва, запропоновано осциляторну модель основного та збудженого станів бозерідини. Подано новий метод врахування ангармонічних членів даного гамільтоніана. Самоузгодженим чином отримано дисперсійне рівняння для колективних збуджень у ⁴Не, де враховано віртуальні та реальні процеси їх розпаду. Отримано точку закінчення спектра, що визначається порогом розпаду колективного збудження на два ротони, та показано, що дисперсійна крива сильно залежить від властивості власної стабільності. Реалізовано підхід із структурним фактором та без використання підгоночних параметрів. Ґрунтуючись на осциляторній моделі запропоновано новий метод самоузгодженого розрахунку енергії основного стану та представлено модель подавлення бозе-конденсату.